

# Effective pseudopotential for energy density functionals with higher order derivatives

F. Raimondi,<sup>1,\*</sup> B. G. Carlsson,<sup>1,2</sup> and J. Dobaczewski<sup>1,3</sup>

<sup>1</sup>*Department of Physics, P.O. Box 35 (YFL) FI-40014 University of Jyväskylä, Finland.*

<sup>2</sup>*Department of Physics, Lund University, P.O. Box 118 Lund 22100, Sweden.*

<sup>3</sup>*Institute of Theoretical Physics, Faculty of Physics,  
University of Warsaw, ul. Hoża 69, PL-00-681 Warsaw, Poland.*

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We derive a zero-range pseudopotential that includes all possible terms up to sixth order in derivatives. Within the Hartree-Fock approximation, it gives the average energy that corresponds to a quasi-local nuclear Energy Density Functional (EDF) built of derivatives of the one-body density matrix up to sixth order. The direct reference of the EDF to the pseudopotential acts as a constraint that divides the number of independent coupling constants of the EDF by two. This allows, e.g., for expressing the isovector part of the functional in terms of the isoscalar part, or *vice versa*. We also derive the analogous set of constraints for the coupling constants of the EDF that is restricted by spherical, space-inversion, and time-reversal symmetries.

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## I. INTRODUCTION

One of the big challenges of the current research in nuclear structure physics is the search for a universal energy density functional (EDF) [1]. Among different possible approaches to this search, the consideration of a local or quasi-local EDF based on the density-matrix expansion (DME) is in recent years the object of intense studies [2–7]. These aim at improving the classic work of Negele and Vautherin [8, 9] and better theoretical understanding based on the effective theory [10, 11] and on the framework of the density functional theory [12].

In the recent work [2], we proposed a new expansion of the nuclear energy density in higher-order derivatives of densities. There, following the effective-theory approach, a Skyrme-like quasi-local next-to-next-to-next-to-leading order ( $N^3LO$ ) EDF was derived with terms of the EDF constrained only by symmetry principles. In the present derivation, we took the route in opposite direction as compared to what has been done for the standard Skyrme next-to-leading order (NLO) EDF. Namely, historically, the Skyrme force has been initially proposed first as an expansion of the effective interaction in relative momenta up to second order [13, 14]. Next, for this force the average Hartree-Fock (HF) energy was evaluated, giving the Skyrme EDF with half of the coupling constants constraint to the other half, see Ref. [15] for the modern complete analysis. Only later, a possibility of releasing these constraints was considered and studied, see, e.g., Ref. [16] for the analysis of the spin-orbit term.

In the present work we complete the results of Ref. [2] by deriving the expansion of the effective interaction in relative momenta up to  $N^3LO$ . This generalizes the Skyrme force up to sixth order and allows us to make a link with the general  $N^3LO$  EDF derived in [2]. One

should stress that the present analysis is not at all an independent repetitive derivation of the same functional. Indeed, the constraints on the EDF coupling constants, which are induced by the HF averaging of this generalized force, cannot be obtained without following the path presented in this study.

The complete higher-order EDFs or pseudopotentials have never yet been applied in practical calculations. The work towards this goal is now in progress, with basic derivations like the ones of Ref. [2] and in the present work coming first, the construction of numerical codes like the one in Ref. [17] coming next, and the full adjustments of coupling constants that will follow. In this respect, at present, we are in a similar phase of studies as before the chiral  $N^3LO$  potentials for two-nucleon systems were adjusted, see, e.g., Ref. [18], and after the tools for calculating the corresponding  $N^3LO$  diagrams were developed, see, e.g., Ref. [19]. Nevertheless, studies of particular higher-order EDF terms have already been performed [20, 21].

In Ref. [22], the question of convergence of the series in higher-order derivatives was recently addressed within the DME applied to the Gogny non-local functional, and it was shown that every next order up to sixth gives contributions smaller by large factors. This gives us confidence that fits of higher-order EDFs have a fair chance of converging. A rigorous power counting scheme, analogous to what has been introduced in the chiral perturbation theory [23], would have to use derivatives of regularized zero-range interactions, see, e.g. Ref. [10]. Such a regularization would provide a proper cut-off scale, against which the powers of derivatives could be estimated. A good model of the regularized delta force is the Gaussian interaction, which, however, leads (through the exchange term) to non-local functionals. Within the EDF methodology, an effective theory based on derivatives of finite-range force is in principle possible, but has not yet been tried because of the degree of numerical complications involved. In the language of the effective field

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\*Electronic address: francesco.raimondi@jyu.fi

theory, the power counting scheme allows us to properly classify diagrams of the perturbation series, however, the ideas of an effective theory are much more general than their applications in the field theory – here we use them within the framework of standard quantum mechanics of many-body systems.

The EDF description of nuclear states is phenomenological in the sense that it depends on the coupling constants, which are usually fitted to available experimental data, see recent Refs. [24, 25] on fitting the second-order (NLO) Skyrme functionals. Fits of the full N<sup>3</sup>LO EDF are much more complicated because of strong interdependencies of the coupling constants and instabilities [26] occurring in certain regions of the parameter space. Our main motivation to carry out the present work was to find constraints on parameters of the general EDF, which result from its relation to a pseudopotential. Such a relation reduces the number of parameters that have to be fit to data, and by this virtue is a positive change, at least at the preliminary stage of adjustments.

Instead of fitting the coupling constants of the EDF, it is also possible to derive them directly using the DME [22]. The DME gives an EDF which approximates more complicated and time consuming HF calculations based on finite-range forces. When applying the DME, the relations to pseudopotentials are however usually broken [4]. By enforcing these relations, as done here, one ensures that the generated EDF is free from unphysical self-interaction [27, 28] and can be applied in beyond-mean-field applications without problems, see, e.g., Refs. [29, 30].

By following the standard convention, here we call the generalized Skyrme force pseudopotential, which is the name denoting a quasi-local operator depending on spatial derivatives. We also consequently use the names ‘parameters’ to denote numerical coefficients of different terms of the pseudopotential, and we use the names ‘coupling constants’ to denote numerical coefficients of terms in the EDF.

The paper is organized as follows. In Sec. II we construct the pseudopotential in two alternative forms and list all its terms up to N<sup>3</sup>LO. We also evaluate the constraints imposed by the gauge symmetry. In Sec. III we discuss the procedure of HF averaging to obtain the EDF from the pseudopotential. In particular, in Sec. III A we derive the general relations connecting the parameters of the Galilean-invariant pseudopotential to the coupling constants of the EDF, whereas in Sec. III B we derive the constraints for the case of conserved gauge symmetry. In Sec. IV we reduce our results to the case of the conserved spherical, space-inversion, and time-reversal symmetries. After formulating the conclusions of the present study in Sec. V, in Appendices A–C we present derivations related to the time-reversal invariance and hermiticity of the pseudopotential, we list results pertaining to the gauge-invariant pseudopotentials, and we give relations between the two alternative forms of pseudopotentials. Results obtained in the present work that are too volu-

minous to be published in the printed form are collected in the supplemental material [31].

## II. GENERAL FORM OF THE PSEUDOPOTENTIAL IN THE SPHERICAL-TENSOR FORMALISM

### A. Central-like form of the pseudopotential

The Skyrme interaction is one of the most important phenomenological effective interaction used in microscopic nuclear structure calculations: such two-body interaction is a short-range expansion up to the second order in derivatives, which contains a certain number of fit parameters adjusted to reproduce the experimental data. In the literature the Skyrme interaction is usually written in cartesian representation, but for our extended pseudopotential we adopt the spherical-tensor representation of operators [32], whose building blocks can be found in [2].

Depending on the specific form of the coupling of the derivative operators with the spin operators, different ways to construct the pseudopotential are possible. A particular form of the pseudopotential, which we call central-like or LS-like, is constructed in the present Section. It is based on coupling together the derivative operators and spin operators, which are then coupled to rotational scalars. An alternative form, called tensor-like or JJ-like, is presented in Section II D. There, each derivative operator is coupled with one spin operator, and then they are coupled together to rotational scalars.

In the central-like form, the pseudopotential is a sum of terms,

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}', \\ \tilde{n}\tilde{L}, v_{12}S}} C_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'} \hat{V}_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'}, \quad (1)$$

where the sum runs over the allowed indices of the tensors according to the symmetries discussed below. Each term in the sum is accompanied by the corresponding strength parameter  $C_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'}$ , and explicitly reads,

$$\begin{aligned} \hat{V}_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'} = & \frac{1}{2} i^{v_{12}} \left( \left[ [K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}]_S \hat{S}_{v_{12}S} \right]_0 \right. \\ & \left. + (-1)^{v_{12}+S} \left[ [K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'}]_S \hat{S}_{v_{12}S} \right]_0 \right) \\ & \times \left( 1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta_{12}(\mathbf{r}'_1 \mathbf{r}'_2; \mathbf{r}_1 \mathbf{r}_2). \end{aligned} \quad (2)$$

In Eq. (2),  $K_{\tilde{n}\tilde{L}}$  are the spherical tensor derivatives of order  $\tilde{n}$  and rank  $\tilde{L}$  built of the spherical representations of the relative momenta  $\mathbf{k} = (\nabla_1 - \nabla_2)/2i$ ,

$$\begin{aligned} k_{1,\mu=\{-1,0,1\}} = & -i \left\{ \frac{1}{\sqrt{2}} (k_x - i k_y), \right. \\ & \left. k_z, \frac{-1}{\sqrt{2}} (k_x + i k_y) \right\}; \end{aligned} \quad (3)$$

TABLE I: Derivative operators  $K_{nL}$  up to N<sup>3</sup>LO as expressed through spherical tensor representation of relative momenta  $k$  defined in Eq. (3).

No.	tensor $K_{nL}$	order $n$	rank $L$
1	1	0	0
2	$k$	1	1
3	$[kk]_0$	2	0
4	$[kk]_2$	2	2
5	$[kk]_0 k$	3	1
6	$[k[kk]_2]_3$	3	3
7	$[kk]_0^2$	4	0
8	$[kk]_0[kk]_2$	4	2
9	$[k[k[kk]_2]_3]_4$	4	4
10	$[kk]_0^2 k$	5	1
11	$[kk]_0[k[kk]_2]_3$	5	3
12	$[k[k[k[kk]_2]_3]_4]_5$	5	5
13	$[kk]_0^3$	6	0
14	$[kk]_0^2[kk]_2$	6	2
15	$[kk]_0[k[k[kk]_2]_3]_4$	6	4
16	$[k[k[k[k[kk]_2]_3]_4]_5]_6$	6	6

up to sixth order they are listed in Table I. Similarly, operators  $K'_{\tilde{n}\tilde{L}}$  are built of the relative momenta  $\mathbf{k}' = (\nabla'_1 - \nabla'_2)/2i$ .

The symmetrized two-body spin operators  $\hat{S}_{v_{12}S}$  are defined as,

$$\hat{S}_{v_{12}S} = (1 - \frac{1}{2}\delta_{v_1, v_2}) \left( [\sigma_{v_1}^{(1)} \sigma_{v_2}^{(2)}]_S + [\sigma_{v_2}^{(1)} \sigma_{v_1}^{(2)}]_S \right), \quad (4)$$

where  $v_{12} = v_1 + v_2$  and  $\sigma_{v\mu}^{(i)}$  are the spherical-tensor components of the rank- $v$  Pauli matrices acting on spin coordinates of particles  $i = 1$  or  $2$ . They are expressed as

$$\sigma_{00}^{(i)} = \hat{1}, \quad (5)$$

$$\sigma_{1,\mu=\{-1,0,1\}}^{(i)} = -i \left\{ \frac{1}{\sqrt{2}} \left( \sigma_x^{(i)} - i\sigma_y^{(i)} \right), \right. \\ \left. \sigma_z^{(i)}, \frac{-1}{\sqrt{2}} \left( \sigma_x^{(i)} + i\sigma_y^{(i)} \right) \right\} \quad (6)$$

through the spin unity matrix  $\hat{1}$  and the standard Cartesian components of the Pauli matrices  $\sigma_{x,y,z}^{(i)}$ .

The Dirac delta function,

$$\hat{\delta}_{12}(\mathbf{r}'_1 \mathbf{r}'_2, \mathbf{r}_1 \mathbf{r}_2) = \delta(\mathbf{r}'_1 - \mathbf{r}_1) \delta(\mathbf{r}'_2 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ = \delta(\mathbf{r}'_1 - \mathbf{r}_2) \delta(\mathbf{r}'_2 - \mathbf{r}_1) \delta(\mathbf{r}_2 - \mathbf{r}_1). \quad (7)$$

ensures the locality and zero-range character of the pseudopotential. The action of derivatives  $K_{\tilde{n}\tilde{L}}$  and  $K'_{\tilde{n}\tilde{L}}$  on  $\hat{\delta}_{12}(\mathbf{r}'_1 \mathbf{r}'_2, \mathbf{r}_1 \mathbf{r}_2)$  has to be understood in the standard sense of derivatives of distributions. Whenever the

pseudopotential (1) is inserted into integrals to calculate the two-body matrix elements, the integration by parts transfers the derivatives onto appropriate wave functions in the remaining parts of integrands.

The exchange term is explicitly embedded in the pseudopotential through the operator

$$\hat{P}^M \hat{P}^\sigma \hat{P}^\tau = (-1)^{\tilde{n}'} \frac{1}{4} \left( 1 + \sqrt{3} \left[ \sigma_1^{(1)} \sigma_1^{(2)} \right]_0 \right. \\ \left. + \sqrt{3} \left[ \tau_1^{(1)} \tau_1^{(2)} \right]^0 + 3 \left[ \sigma_1^{(1)} \sigma_1^{(2)} \right]_0 \left[ \tau_1^{(1)} \tau_1^{(2)} \right]^0 \right), \quad (8)$$

where  $\tau_1^{(i)}$  are the standard spherical-tensor isospin Pauli matrices defined analogously as in Eq. (6). The square brackets with superscripts and subscripts denote the coupling of spherical tensors in the isospin space and coordinate space, respectively. The above definitions and conventions exactly correspond to those introduced in Ref. [2].

The zero range of the pseudopotential has an important bearing on the structure of terms in Eq. (2). Indeed, only for the zero-range force, the space-exchange (Majorana) operator  $\hat{P}^M$  can be replaced, in any individual term, by the phase  $(-1)^{\tilde{n}'}$  appearing in Eq. (8). Moreover, apart from the isospin-exchange operator  $\hat{P}^\tau$ , terms of the pseudopotential cannot then depend on isospin. This fact, effectively reduces by half the number of allowed terms of the pseudopotential, as compared to what would have been possible for a finite-range potential. This is at the origin of the numbers of allowed terms of the pseudopotential being equal one half of the numbers of the allowed terms of the EDF, which we discuss below.

The full antisymmetrization of the pseudopotential includes the exchange operator in the isospin space; therefore, in the following we consider the EDF with the isospin degree of freedom included, that is, we discuss both the isoscalar and isovector terms of the N<sup>3</sup>LO [2], which allows us to fully incorporate the proton-neutron mixing at the level of the energy density [15].

The general form of the pseudopotential and the allowed terms listed below reflect the fact that the fundamental symmetries of the two-body interaction must be respected, see Appendix A. In particular, (i) all terms are scalar operators, that is, they are coupled to the total angular momentum 0, which ensures the rotational invariance, (ii) the total number of derivative operators must be even, namely,  $\tilde{n} + \tilde{n}' = 0, 2, 4, 6$ , which ensures the time-reversal and parity invariances, (iii) the parameters  $C_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'}$  of the pseudopotential must be real, to guarantee both the time-reversal invariance and hermiticity, and (iv) the invariance under exchange of the coordinates of particle 1 and 2 is respected by expression (2).

TABLE II: Zero-order terms of the pseudopotential (2).

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$S$	gauge
1	0	0	0	0	0	0	Y
2	0	0	0	0	2	0	Y

TABLE III: Same as in Table II but for the second order terms.

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$S$	gauge
1	2	0	0	0	0	0	Y
2	2	0	0	0	2	0	Y
3	2	2	0	0	2	2	Y
4	1	1	1	1	0	0	Y
5	1	1	1	1	2	0	Y
6	1	1	1	1	1	1	Y
7	1	1	1	1	2	2	Y

### B. Lists of terms of the pseudopotential $\hat{V}$ order by order

In Tables II-V are listed, respectively, all possible terms of the pseudopotential (1) in zero, second, fourth, and sixth order. In each order, the numbers of terms equal 2, 7, 15, and 26, giving the total number of 50 terms up to N<sup>3</sup>LO. We see that these numbers of terms are exactly equal to those corresponding to the EDF in *each* isospin channel with the Galilean invariance imposed, cf. Table VI of Ref. [2]. One should note that each term of the pseudopotential (2) is Galilean-invariant by construction, because it is built with relative-momentum operators  $K_{\tilde{n}\tilde{L}}$ ; therefore, the pseudopotential is not changed by a transformation to a system moving with a constant velocity. When both isoscalar and isovector channels are considered in the EDF, the number of EDF terms becomes in each order *twice larger* than the number of terms of the pseudopotential.

This means that the EDF obtained by averaging the pseudopotential is constrained by as many conditions as there are terms in each isospin channel. One possible solution is than to find a one-to-one correspondence between the EDF and the pseudopotential by relating the isoscalar part of the EDF to its isovector part, in a way that will be showed explicitly in the following Sections of this work.

To make the connection between the pseudopotential and the standard form of the Skyrme interaction more transparent, we give here the relations of conversion between the parameters of the zero- and second-order pseudopotential and those of the Skyrme interaction, see

TABLE IV: Same as in Table II but for the fourth order terms.

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$S$	gauge
1	4	0	0	0	0	0	D
2	4	0	0	0	2	0	D
3	4	2	0	0	2	2	D
4	3	1	1	1	0	0	Y
5	3	1	1	1	2	0	Y
6	3	1	1	1	1	1	N
7	3	1	1	1	2	2	D
8	3	3	1	1	2	2	I
9	2	0	2	0	0	0	D
10	2	0	2	0	2	0	D
11	2	2	2	0	2	2	D
12	2	2	2	2	0	0	I
13	2	2	2	2	2	0	I
14	2	2	2	2	1	1	N
15	2	2	2	2	2	2	I

Ref. [15] for the definitions used. They read,

$$t_0 = C_{00,00}^{00} + \frac{1}{\sqrt{3}}C_{00,20}^{00}, \quad (9a)$$

$$t_0x_0 = -\frac{2}{\sqrt{3}}C_{00,20}^{00}, \quad (9b)$$

$$t_1 = \frac{1}{\sqrt{3}}C_{00,00}^{20} + \frac{1}{3}C_{00,20}^{20}, \quad (9c)$$

$$t_1x_1 = -\frac{2}{3}C_{00,20}^{20}, \quad (9d)$$

$$t_2 = \frac{1}{\sqrt{3}}C_{11,00}^{11} + \frac{1}{3}C_{11,20}^{11}, \quad (9e)$$

$$t_2x_2 = -\frac{2}{3}C_{11,20}^{11}, \quad (9f)$$

$$W_0 = \frac{1}{\sqrt{6}}C_{11,11}^{11}, \quad (9g)$$

$$t_o = -\frac{1}{3\sqrt{5}}C_{11,22}^{11}, \quad (9h)$$

$$t_e = -\frac{1}{3\sqrt{5}}C_{00,22}^{22}. \quad (9i)$$

In relations of Eqs. (9), parameters  $t_3$  and  $t_3x_3$  are missing: they are related to the terms of the Skyrme interaction depending on density, which have been introduced to mimic the effects of the three-body force in the phenomenological interaction and to get the saturation feature of the nuclear force. In the same way, the zero-order parameters  $C_{00,00}^{00}$  and  $C_{00,20}^{00}$  of the pseudopotential, see Eqs. (9a) and (9b), should become density-dependent.

In his effective nuclear potential, Skyrme also introduced [14] one additional term of the fourth order, which he justified through the presence of considerable D-waves in the nucleon-nucleon interaction energies around

TABLE V: Same as in Table II but for the sixth order terms.

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$S$	gauge
1	6	0	0	0	0	0	D
2	6	0	0	0	2	0	D
3	6	2	0	0	2	2	D
4	5	1	1	1	0	0	D
5	5	1	1	1	2	0	D
6	5	1	1	1	1	1	N
7	5	1	1	1	2	2	D
8	5	3	1	1	2	2	I
9	4	0	2	0	0	0	D
10	4	0	2	0	2	0	D
11	4	2	2	0	2	2	D
12	4	0	2	2	2	2	D
13	4	2	2	2	0	0	I
14	4	2	2	2	2	0	I
15	4	2	2	2	1	1	N
16	4	2	2	2	2	2	D
17	4	4	2	2	2	2	I
18	3	1	3	1	0	0	D
19	3	1	3	1	2	0	D
20	3	1	3	1	1	1	N
21	3	1	3	1	2	2	D
22	3	3	3	1	2	2	D
23	3	3	3	3	0	0	I
24	3	3	3	3	2	0	I
25	3	3	3	3	1	1	N
26	3	3	3	3	2	2	D

100 MeV. Also in this case, we give the relation between the corresponding parameter  $t_D$  and the parameter of our full pseudopotential,

$$t_D = \frac{1}{2} C_{20,20}^{00}. \quad (10)$$

### C. Gauge invariance of the pseudopotential

Besides the Galilean invariance mentioned above, the standard Skyrme force has been also proved to be invariant with respect to a more general local gauge invariance, and to give rise to the energy density that is invariant under the same symmetry when specific relations between the coupling constants are set [33, 34].

The gauge transformation acts on a many-body wave function by multiplying it with a position-dependent

phase factor, that is,

$$|\Psi'\rangle = \exp\left(i \sum_{j=1}^A \phi(r_j)\right) |\Psi\rangle, \quad (11)$$

and its action transferred onto the pseudopotential is,

$$\hat{V}' = e^{-i\phi(r'_2)} e^{-i\phi(r'_1)} \hat{V} e^{i\phi(r_1)} e^{i\phi(r_2)}. \quad (12)$$

Apart from zero order, the terms of the pseudopotential are not trivially invariant with respect to the transformation of the Eq. (12) and, in general, the transformed pseudopotential  $\hat{V}'$  is different than the original pseudopotential  $\hat{V}$ . To impose the gauge invariance on the pseudopotential, one has to derive a list of constraints among the parameters, which can be done using the condition

$$[\phi(r_1), \hat{V}] + [\phi(r_2), \hat{V}] = 0. \quad (13)$$

As expected, at second order, all the 7 terms of the pseudopotential listed in Table III fulfill condition (13). Then they all are the stand-alone gauge invariant terms of the pseudopotential, which in the last column of the Table is marked by the letter Y. On the other hand, at fourth order, only two of the terms of the pseudopotential listed in Table IV, those that correspond to parameters  $C_{11,00}^{31}$  and  $C_{11,20}^{31}$ , fulfill condition (13). At sixth order, none of the terms are stand-alone gauge invariant.

At fourth order, the gauge invariance forces seven parameters of the pseudopotential to be specific linear combinations of four independent ones. In Table IV, they are marked by letters D and I, respectively. In Appendix B, we list such relations between the dependent and independent parameters. One should note that other choices of the four independent parameters are also possible, that is, at fourth order, there are simply four different gauge-invariant linear combinations of terms of the pseudopotential (1). Moreover, at this order, there are also two terms that alone are gauge non-invariant – those that correspond to parameters  $C_{11,11}^{31}$  and  $C_{22,11}^{22}$ ; in Table IV, they are marked by letters N. Similarly, at sixth order, there are six gauge-invariant linear combinations of terms of the pseudopotential, that is, sixteen dependent parameters are related to six independent ones, see Appendix B, and there are also four alone gauge non-invariant terms corresponding to parameters  $C_{11,11}^{51}$ ,  $C_{22,11}^{42}$ ,  $C_{31,11}^{31}$ , and  $C_{33,11}^{33}$ .

A comparison between the numbers of terms of the Galilean-invariant pseudopotential and the gauge-invariant pseudopotential is plotted in Fig. 1. Again we note that at each order, the numbers of gauge-invariant parameters (2 for the zero order, 7 for the second order, 6 for the fourth order, and 6 for the sixth order) are exactly the same as the numbers of independent coupling constants of the EDF in *each* isospin channel with the gauge invariance imposed, cf. Table VI of Ref. [2]. Again, this observation will be crucial when we proceed to derive

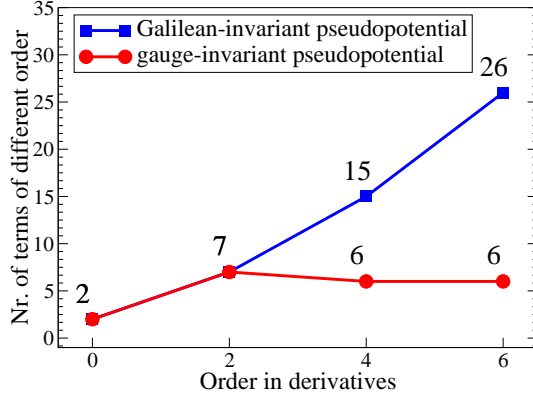


FIG. 1: (Color online) Number of terms of the pseudopotential (2), plotted as a function of the order in derivatives.

relations between the isoscalar and the isovector parts of the EDF, stemming from the gauge-invariant pseudopotential. We also remark that whereas the second-order spin-orbit term, corresponding to parameter  $C_{11,11}^{11}$ , is gauge invariant, all higher-order spin-orbit terms, corresponding to parameters  $C_{\tilde{n}\tilde{L},11}^{\tilde{n}'\tilde{L}'}$  with  $\tilde{n} + \tilde{n}' > 2$  do violate the gauge symmetry.

#### D. Tensor-like form of the pseudopotential

In this Section, we present the tensor-like form of the pseudopotential, which is, in fact, a different form of coupling of the relative-momentum operators with the spin operators, just like in the tensor term of the standard Skyrme interaction. In this form, the pseudopotential of Eq. (1) is a sum of the following terms,

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}', \\ \tilde{n}\tilde{L}, v_{12}J}} \tilde{C}_{\tilde{n}\tilde{L}, v_{12}J}^{\tilde{n}'\tilde{L}'} \hat{V}_{\tilde{n}\tilde{L}, v_{12}J}^{\tilde{n}'\tilde{L}'} \quad (14)$$

where

$$\begin{aligned} \hat{V}_{\tilde{n}\tilde{L}, v_{12}J}^{\tilde{n}'\tilde{L}'} = & \frac{1}{2} i^{v_{12}} \left( 1 - \frac{1}{2} \delta_{v_1, v_2} \right) \times \\ & \left( \left[ \left[ K'_{\tilde{n}'\tilde{L}'} \sigma_{v_1}^{(1)} \right]_J \left[ K_{\tilde{n}\tilde{L}} \sigma_{v_2}^{(2)} \right]_J \right]_0 \right. \\ & + \left[ \left[ K'_{\tilde{n}'\tilde{L}'} \sigma_{v_1}^{(2)} \right]_J \left[ K_{\tilde{n}\tilde{L}} \sigma_{v_2}^{(1)} \right]_J \right]_0 \\ & + \left[ \left[ K'_{\tilde{n}\tilde{L}} \sigma_{v_1}^{(1)} \right]_J \left[ K_{\tilde{n}'\tilde{L}'} \sigma_{v_2}^{(2)} \right]_J \right]_0 \\ & \left. + \left[ \left[ K'_{\tilde{n}\tilde{L}} \sigma_{v_1}^{(2)} \right]_J \left[ K_{\tilde{n}'\tilde{L}'} \sigma_{v_2}^{(1)} \right]_J \right]_0 \right) \times \\ & \left( 1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta_{12}(\mathbf{r}'_1 \mathbf{r}'_2; \mathbf{r}_1 \mathbf{r}_2). \quad (15) \end{aligned}$$

The lists of the zero-, second-, fourth-, and sixth-order terms  $\hat{V}_{\tilde{n}\tilde{L}, v_{12}J}^{\tilde{n}'\tilde{L}'}$  of the pseudopotential are given, respectively, in Tables VI–IX, which are the analogues of Tables II–V given in Section II B.

TABLE VI: Zero-order terms of the recoupled pseudopotential (15).

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$J$
1	0	0	0	0	0	0
2	0	0	0	0	2	0

TABLE VII: Same as in Table VI but for the second-order terms.

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$J$
1	1	1	1	1	0	1
2	1	1	1	1	1	1
3	1	1	1	1	2	0
4	1	1	1	1	2	1
5	1	1	1	1	2	2
6	2	0	0	0	0	0
7	2	0	0	0	2	1
8	2	2	0	0	2	1

By means of the recoupling technique, it is possible to determine relations between the two different coupling schemes of the pseudopotential. This derivation, along with the relationships between the corresponding parameters  $C_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'}$  and  $\tilde{C}_{\tilde{n}\tilde{L}, v_{12}J}^{\tilde{n}'\tilde{L}'}$ , is presented in Appendix C.

TABLE VIII: Same as in Table VI but for the fourth-order terms.

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$J$
1	2	0	2	0	0	0
2	2	0	2	0	2	1
3	2	2	2	2	0	2
4	2	2	2	2	1	2
5	2	2	2	0	2	1
6	2	2	2	2	2	1
7	2	2	2	2	2	2
8	2	2	2	2	2	3
9	3	1	1	1	0	1
10	3	1	1	1	1	1
11	3	1	1	1	2	0
12	3	1	1	1	2	1
13	3	1	1	1	2	2
14	3	3	1	1	2	2
15	4	0	0	0	0	0
16	4	0	0	0	2	1
17	4	2	0	0	2	1

TABLE IX: Same as in Table VI but for the sixth-order terms.

No.	$\tilde{n}'$	$\tilde{L}'$	$\tilde{n}$	$\tilde{L}$	$v_{12}$	$J$
1	3	1	3	1	0	1
2	3	1	3	1	1	1
3	3	1	3	1	2	0
4	3	1	3	1	2	1
5	3	1	3	1	2	2
6	3	3	3	3	0	3
7	3	3	3	3	1	3
8	3	3	3	1	2	2
9	3	3	3	3	2	2
10	3	3	3	3	2	3
11	3	3	3	3	2	4
12	4	0	2	0	0	0
13	4	0	2	0	2	1
14	4	0	2	2	2	1
15	4	2	2	2	0	2
16	4	2	2	2	1	2
17	4	2	2	0	2	1
18	4	2	2	2	2	1
19	4	2	2	2	2	2
20	4	2	2	2	2	3
21	4	4	2	2	2	3
22	5	1	1	1	0	1
23	5	1	1	1	1	1
24	5	1	1	1	2	0
25	5	1	1	1	2	1
26	5	1	1	1	2	2
27	5	3	1	1	2	2
28	6	0	0	0	0	0
29	6	0	0	0	2	1
30	6	2	0	0	2	1

The reader might have noticed that the two forms of the pseudopotential do not have the same numbers of

terms: the tensor-like form of the pseudopotential (Tables VII, VIII, and IX) has more terms than the central-like form (Tables III, IV, and V). This means that not all of the terms of the tensor-like form are linearly independent from one another, even though they are all allowed by the symmetries, and thus some terms can be expressed as linear combinations of others, or, equivalently, some linear combinations of terms are identically equal to zero. This fact, can be expressed in the form of the following explicit dependencies between the parameters of the tensor-like pseudopotential.

For the second-order terms we have,

$$\tilde{C}_{11,21}^{11} = -\frac{2}{\sqrt{3}}\tilde{C}_{11,20}^{11} + \sqrt{\frac{5}{3}}\tilde{C}_{11,22}^{11}, \quad (16)$$

whereas the fourth-order dependencies read,

$$\tilde{C}_{22,21}^{22} = -\frac{\sqrt{15}}{9}\tilde{C}_{22,22}^{22} + \frac{2}{9}\sqrt{21}\tilde{C}_{22,23}^{22}, \quad (17a)$$

$$\tilde{C}_{11,21}^{31} = -\frac{2}{\sqrt{3}}\tilde{C}_{11,20}^{31} + \sqrt{\frac{5}{3}}\tilde{C}_{11,22}^{31}, \quad (17b)$$

and finally at sixth order we have,

$$\tilde{C}_{31,21}^{31} = -\frac{2}{\sqrt{3}}\tilde{C}_{31,20}^{31} + \sqrt{\frac{5}{3}}\tilde{C}_{31,22}^{31}, \quad (18a)$$

$$\tilde{C}_{33,23}^{33} = -4\sqrt{\frac{5}{7}}\tilde{C}_{33,22}^{33} + \frac{9}{\sqrt{7}}\tilde{C}_{33,24}^{33}, \quad (18b)$$

$$\tilde{C}_{22,21}^{42} = -\frac{\sqrt{15}}{9}\tilde{C}_{22,22}^{42} + \frac{2}{9}\sqrt{21}\tilde{C}_{22,23}^{42}, \quad (18c)$$

$$\tilde{C}_{11,21}^{51} = -\frac{2}{\sqrt{3}}\tilde{C}_{11,20}^{51} + \sqrt{\frac{5}{3}}\tilde{C}_{11,22}^{51}. \quad (18d)$$

### III. RELATIONS BETWEEN THE PSEUDOPOTENTIAL AND ENERGY DENSITY FUNCTIONAL

The EDF related to the pseudopotential is obtained by averaging the pseudopotential  $\hat{V}$  over the uncorrelated wavefunction (a Slater determinant), that is,

$$\mathcal{E} = \frac{1}{4} \int d\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}'_1 \mathbf{r}'_2 \sum_{\substack{s_1 s_2 t_1 t_2 \\ s'_1 s'_2 t'_1 t'_2}} \hat{V}(\mathbf{r}'_1 s'_1 t'_1 \mathbf{r}'_2 s'_2 t'_2, \mathbf{r}_1 s_1 t_1 \mathbf{r}_2 s_2 t_2) \rho(\mathbf{r}_1 s_1 t_1, \mathbf{r}'_1 s'_1 t'_1) \rho(\mathbf{r}_2 s_2 t_2, \mathbf{r}'_2 s'_2 t'_2), \quad (19)$$

where the two-body spin-isospin matrix element of the pseudopotential is defined as

$$\hat{V}(\mathbf{r}'_1 s'_1 t'_1 \mathbf{r}'_2 s'_2 t'_2, \mathbf{r}_1 s_1 t_1 \mathbf{r}_2 s_2 t_2) = \langle s'_1 t'_1, s'_2 t'_2 | \hat{V} | s_1 t_1, s_2 t_2 \rangle, \quad (20)$$

and  $\rho(\mathbf{r}_1 s_1 t_1, \mathbf{r}'_1 s'_1 t'_1)$  and  $\rho(\mathbf{r}_2 s_2 t_2, \mathbf{r}'_2 s'_2 t'_2)$ , are the one-body densities in spin-isospin channels. (For definitions,

see, e.g., Ref. [15].) In this lengthy calculation, one must consider as intermediate step the recoupling of the

TABLE X: Second-order coupling constants of the isoscalar EDF ( $t = 0$ ) as functions of parameters of the pseudopotential, expressed by the formula  $C_{mI,nLvJ}^{n'L'v'J',0} = A(aC_{00,00}^{20} + bC_{00,20}^{20} + cC_{00,22}^{22} + dC_{11,00}^{11} + eC_{11,20}^{11} + fC_{11,11}^{11} + gC_{11,22}^{11})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$C_{20,0000}^{0000,0}$	$\frac{1}{32}$	-3	$-\sqrt{3}$	0	5	$-\sqrt{3}$	0	0
$C_{00,2000}^{0000,0}$	$\frac{1}{16}$	3	$\sqrt{3}$	0	5	$-\sqrt{3}$	0	0
$C_{00,1110}^{1110,0}$	$\frac{1}{48}$	$\sqrt{3}$	5	$2\sqrt{5}$	$-\sqrt{3}$	3	0	$6\sqrt{5}$
$C_{00,1111}^{1111,0}$	$\frac{1}{48}$	3	$5\sqrt{3}$	$-\sqrt{15}$	-3	$3\sqrt{3}$	0	$-3\sqrt{15}$
$C_{00,1112}^{1112,0}$	$\frac{1}{48}$	$\sqrt{15}$	$5\sqrt{5}$	1	$-\sqrt{15}$	$3\sqrt{5}$	0	3
$C_{11,1111}^{0000,0}$	$-\frac{3}{4}$	0	0	0	0	0	1	0
$C_{00,1101}^{1101,0}$	$\frac{1}{16}$	-3	$-\sqrt{3}$	0	-5	$\sqrt{3}$	0	0
$C_{20,0011}^{0011,0}$	$\frac{1}{32}$	$\sqrt{3}$	5	0	$\sqrt{3}$	-3	0	0
$C_{22,0011}^{0011,0}$	$\frac{1}{16}$	0	0	1	0	0	0	-3
$C_{00,2011}^{0011,0}$	$\frac{1}{16}$	$-\sqrt{3}$	-5	0	$\sqrt{3}$	-3	0	0
$C_{00,2211}^{0011,0}$	$\frac{1}{8}$	0	0	-1	0	0	0	-3
$C_{11,0011}^{1101,0}$	$-\frac{3}{4}$	0	0	0	0	0	1	0

relative-momentum operators, so as to recast the gradients in such a way that each tensor affects only one particle at a time [15]. Such recoupling was performed with the aid of symbolic programming, and is not, for the sake of brevity, reported in this paper.

For each term of the pseudopotential (1), we can write the result of the averaging in the following way,

$$\langle C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} \hat{V}_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} \rangle = \sum C_{mI,nLvJ}^{n'L'v'J',t} T_{mI,nLvJ}^{n'L'v'J',t}, \quad (21)$$

where  $C_{mI,nLvJ}^{n'L'v'J',t}$  and  $T_{mI,nLvJ}^{n'L'v'J',t}$  denote, respectively, the coupling constants and terms of the EDF according to the formalism developed in Ref. [2]. Since here we treat the isospin degree of freedom explicitly, to the notation of Ref. [2] we have added superscripts  $t$ , which denote the isoscalar ( $t = 0$ ) and isovector ( $t = 1$ ) channels.

Once relations (21) are evaluated for each term of the pseudopotential, all terms of the N<sup>3</sup>LO EDF are generated, with the EDF coupling constants  $C_{mI,nLvJ}^{n'L'v'J',t}$  becoming linear combinations of the pseudopotential strength parameters  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'}$ . Since the pseudopotentials are Galilean-invariant, the obtained EDF coupling constants obey the Galilean-invariance constraints [2]. Similarly, when parameters of the pseudopotential are restricted to obey the gauge-invariance conditions defined in Sec. II C, the resulting coupling constants correspond to a gauge-invariant EDF.

The 12 second-order isoscalar (isovector) coupling constants expressed by the 7 second-order pseudopotential parameters are given in Table X (Table XI). Similar expressions relating at fourth (sixth) order 45 (129) isoscalar and isovector coupling constants to 15 (26) pseudopotential parameters, are available in the supplemental material [31].

TABLE XI: Same as in Table X but for isovector EDF ( $t = 1$ ), according to the formula  $C_{mI,nLvJ}^{n'L'v'J',1} = A(aC_{00,00}^{20} + bC_{00,20}^{20} + cC_{00,22}^{22} + dC_{11,00}^{11} + eC_{11,20}^{11} + fC_{11,11}^{11} + gC_{11,22}^{11})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$C_{20,0000}^{0000,1}$	$\frac{1}{32}$	$\sqrt{3}$	-3	0	$\sqrt{3}$	-3	0	0
$C_{00,2000}^{0000,1}$	$\frac{1}{16}$	$-\sqrt{3}$	3	0	$\sqrt{3}$	-3	0	0
$C_{00,1110}^{1110,1}$	$\frac{1}{48}$	3	$\sqrt{3}$	$-2\sqrt{15}$	-3	$-\sqrt{3}$	0	$2\sqrt{15}$
$C_{00,1111}^{1111,1}$	$\frac{1}{16}$	$\sqrt{3}$	1	$\sqrt{5}$	$-\sqrt{3}$	-1	0	$-\sqrt{5}$
$C_{00,1112}^{1112,1}$	$\frac{1}{48}$	$3\sqrt{5}$	$\sqrt{15}$	$-\sqrt{3}$	$-3\sqrt{5}$	$-\sqrt{15}$	0	$\sqrt{3}$
$C_{11,1111}^{0000,1}$	$-\frac{1}{4}\sqrt{3}$	0	0	0	0	0	1	0
$C_{00,1101}^{1101,1}$	$\frac{1}{16}$	$\sqrt{3}$	-3	0	$-\sqrt{3}$	3	0	0
$C_{20,0011}^{0011,1}$	$\frac{1}{32}$	3	$\sqrt{3}$	0	3	$\sqrt{3}$	0	0
$C_{22,0011}^{0011,1}$	$-\frac{1}{16}\sqrt{3}$	0	0	1	0	0	0	1
$C_{00,2011}^{0011,1}$	$\frac{1}{16}$	-3	$-\sqrt{3}$	0	3	$\sqrt{3}$	0	0
$C_{00,2211}^{0011,1}$	$\frac{1}{8}\sqrt{3}$	0	0	1	0	0	0	-1
$C_{11,0011}^{1101,1}$	$-\frac{1}{4}\sqrt{3}$	0	0	0	0	0	1	0

### A. Inverse relations

In Section II we noticed the fact that once either the Galilean or gauge invariance is imposed, the numbers of parameters of the pseudopotential are the same, at each order, as the numbers of coupling constants of the EDF for *each* isospin. This situation allows us to obtain the inverse relations, namely, expressions relating the coupling constants of the EDF to the parameters of the pseudopotential. For the case of gauge invariance, at second order they are given in Tables XII and XIII, at fourth order in Tables XIV and XV, and at sixth order in Tables XVI and XVII. As sets of independent coupling constants of the gauge-invariant EDF we selected the ones used in Appendix C of Ref. [2]. Note that in each case, the parameters of the pseudopotential can be expressed either by the isoscalar or by the isovector coupling constants. For the case of Galilean invariance, analogous expressions are available in the supplemental material [31].

### B. Constraints on the Energy Density Functional

The zero range of the pseudopotential is at the origin of the specific constraints induced upon the resulting coupling constants of the EDF. Indeed, elimination of the pseudopotential parameters from pairs of relationships defined by Tables XII–XIII, XIV–XV, and XVI–XVII leaves us with sets of linear equations that the EDF coupling constants must obey. At second order, that is, for the standard Skyrme interaction, this fact is well known and allows us to express the time-odd coupling constants through the time-even ones, see Ref. [4] for the complete set of expressions. We do not yet know if the analogous property may hold at higher orders, because this fact crucially depend on the arbitrary choice of the indepen-



TABLE XII: Second-order parameters of the pseudopotential as functions of the coupling constants of the isoscalar EDF ( $t = 0$ ) when the gauge invariance is imposed, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = A(aC_{20,0000}^{0000,0} + bC_{20,0011}^{0011,0} + cC_{22,0011}^{0011,0} + dC_{00,1101}^{1101,0} + eC_{11,0011}^{1101,0} + fC_{00,2011}^{0011,0} + gC_{00,2211}^{0011,0})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$C_{00,00}^{20}$	$-\frac{2}{3}$	10	$2\sqrt{3}$	0	5	0	$-\sqrt{3}$	0
$C_{00,20}^{20}$	$\frac{2}{3}$	$2\sqrt{3}$	6	0	$\sqrt{3}$	0	-3	0
$C_{00,22}^{22}$	-4	0	0	-2	0	0	0	1
$C_{11,00}^{11}$	$-\frac{2}{3}$	-6	$2\sqrt{3}$	0	3	0	$\sqrt{3}$	0
$C_{11,20}^{11}$	$-\frac{2}{3}$	$-2\sqrt{3}$	10	0	$\sqrt{3}$	0	5	0
$C_{11,11}^{11}$	$-\frac{4}{3}$	0	0	0	0	1	0	0
$C_{11,22}^{11}$	$-\frac{4}{3}$	0	0	2	0	0	0	1

TABLE XIII: Same as in Table XII but for the isovector EDF ( $t = 1$ ), according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = A(aC_{20,0000}^{0000,1} + bC_{20,0011}^{0011,1} + cC_{22,0011}^{0011,1} + dC_{00,1101}^{1101,1} + eC_{11,0011}^{1101,1} + fC_{00,2011}^{0011,1} + gC_{00,2211}^{0011,1})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$C_{00,00}^{20}$	$\frac{2}{3}$	$2\sqrt{3}$	6	0	$\sqrt{3}$	0	-3	0
$C_{00,20}^{20}$	$-\frac{2}{3}$	6	$-2\sqrt{3}$	0	3	0	$\sqrt{3}$	0
$C_{00,22}^{22}$	$\frac{4}{3}$	0	0	$-2\sqrt{3}$	0	0	0	$\sqrt{3}$
$C_{11,00}^{11}$	$-\frac{2}{3}$	$-2\sqrt{3}$	-6	0	$\sqrt{3}$	0	-3	0
$C_{11,20}^{11}$	$\frac{2}{\sqrt{3}}$	$-2\sqrt{3}$	2	0	$\sqrt{3}$	0	1	0
$C_{11,11}^{11}$	$-\frac{4}{\sqrt{3}}$	0	0	0	0	1	0	0
$C_{11,22}^{11}$	$-\frac{4}{\sqrt{3}}$	0	0	2	0	0	0	1

dent coupling constants that define the Galilean or gauge symmetries.

In the present paper, we derive the set of constraints on the EDF coupling constants that can be obtained by inverting the relations for the isovector coupling constants, given in Tables XIII, XV, and XVII. This allows us to

TABLE XIV: Same as in Table XII but for the fourth-order parameters of the pseudopotential, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = A(aC_{00,2202}^{2202,0} + bC_{00,2212}^{2212,0} + cC_{00,4211}^{0011,0} + dC_{40,0000}^{0000,0} + eC_{40,0011}^{0011,0} + fC_{42,0011}^{0011,0})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{11,00}^{31}$	$\frac{2}{15}$	$18\sqrt{5}$	$-18\sqrt{5}$	$-7\sqrt{15}$	-120	$40\sqrt{3}$	0
$C_{11,20}^{31}$	$\frac{2}{15}$	$6\sqrt{15}$	$-30\sqrt{15}$	$-35\sqrt{5}$	$-40\sqrt{3}$	200	0
$C_{11,22}^{33}$	$\frac{8}{3}\sqrt{\frac{7}{15}}$	0	0	-1	0	0	2
$C_{22,00}^{22}$	$\frac{1}{9}$	30	18	$7\sqrt{3}$	$40\sqrt{5}$	$8\sqrt{15}$	0
$C_{22,20}^{22}$	$-\frac{1}{9\sqrt{5}}$	$6\sqrt{15}$	$18\sqrt{15}$	$21\sqrt{5}$	$40\sqrt{3}$	120	0
$C_{22,22}^{22}$	$-\frac{4}{3}\sqrt{7}$	0	0	1	0	0	2

TABLE XV: Same as in Table XIII but for the fourth-order parameters of the pseudopotential, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = A(aC_{00,2202}^{2202,1} + bC_{00,2212}^{2212,1} + cC_{00,4211}^{0011,1} + dC_{40,0000}^{0000,1} + eC_{40,0011}^{0011,1} + fC_{42,0011}^{0011,1})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{11,00}^{31}$	$-\frac{2}{15}$	$-6\sqrt{15}$	$-18\sqrt{15}$	$-21\sqrt{5}$	$40\sqrt{3}$	120	0
$C_{11,20}^{31}$	$-\frac{2}{15}$	$18\sqrt{5}$	$-18\sqrt{5}$	$-7\sqrt{15}$	-120	$40\sqrt{3}$	0
$C_{11,22}^{33}$	$\frac{8}{3}\sqrt{\frac{7}{5}}$	0	0	-1	0	0	2
$C_{22,00}^{22}$	$\frac{1}{9}$	$-6\sqrt{3}$	$-18\sqrt{3}$	-21	$-8\sqrt{15}$	$-24\sqrt{5}$	0
$C_{22,20}^{22}$	$\frac{1}{9\sqrt{5}}$	$18\sqrt{5}$	$-18\sqrt{5}$	$-7\sqrt{15}$	120	$-40\sqrt{3}$	0
$C_{22,22}^{22}$	$\frac{4}{3}\sqrt{\frac{7}{3}}$	0	0	1	0	0	2

TABLE XVI: Same as in Table XII but for the sixth-order parameters of the pseudopotential, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = A(aC_{00,4212}^{2212,0} + bC_{00,3303}^{3303,0} + cC_{00,6211}^{0011,0} + dC_{60,0000}^{0000,0} + eC_{60,0011}^{0011,0} + fC_{62,0011}^{0011,0})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{11,22}^{53}$	$-\frac{16}{3}\sqrt{\frac{7}{15}}$	0	0	1	0	0	2
$C_{22,00}^{42}$	$\frac{2}{21}$	21	$-15\sqrt{105}$	$42\sqrt{3}$	$-208\sqrt{5}$	$-56\sqrt{15}$	0
$C_{22,20}^{42}$	$-\frac{2}{3}\sqrt{\frac{1}{7}}$	$3\sqrt{21}$	$-9\sqrt{5}$	$18\sqrt{7}$	$-8\sqrt{105}$	$-24\sqrt{35}$	0
$C_{22,22}^{44}$	$-\frac{16}{\sqrt{5}}$	0	0	1	0	0	-2
$C_{33,00}^{33}$	$-\frac{2}{45}$	$\sqrt{105}$	45	$6\sqrt{35}$	$-40\sqrt{21}$	$40\sqrt{7}$	0
$C_{33,20}^{33}$	$\frac{2}{9}\sqrt{\frac{1}{15}}$	$-5\sqrt{21}$	$-9\sqrt{5}$	$-30\sqrt{7}$	$8\sqrt{105}$	$-40\sqrt{35}$	0

express, at each order, the isovector coupling constants through the isoscalar ones. For the case of gauge invariance, at second, fourth, and sixth order, such relations are listed in Tables XVIII, XIX, and XX, respectively. For the case of Galilean invariance, analogous expressions are available in the supplemental material [31].

TABLE XVII: Same as in Table XIII but for the sixth-order parameters of the pseudopotential, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = A(aC_{00,4212}^{2212,1} + bC_{00,3303}^{3303,1} + cC_{00,6211}^{0011,1} + dC_{60,0000}^{0000,1} + eC_{60,0011}^{0011,1} + fC_{62,0011}^{0011,1})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{11,22}^{53}$	$-\frac{16}{3}\sqrt{\frac{7}{5}}$	0	0	1	0	0	2
$C_{22,00}^{42}$	$\frac{2}{7\sqrt{3}}$	-21	$3\sqrt{105}$	$-42\sqrt{3}$	$56\sqrt{5}$	$56\sqrt{15}$	0
$C_{22,20}^{42}$	$-\frac{2}{21}$	21	$9\sqrt{105}$	$42\sqrt{3}$	$168\sqrt{5}$	$-56\sqrt{15}$	0
$C_{22,22}^{44}$	$\frac{16}{\sqrt{15}}$	0	0	1	0	0	-2
$C_{33,00}^{33}$	$-\frac{2}{45}$	$-3\sqrt{35}$	$15\sqrt{3}$	$-6\sqrt{105}$	$-40\sqrt{7}$	$-40\sqrt{21}$	0
$C_{33,20}^{33}$	$\frac{2}{9}\sqrt{\frac{1}{15}}$	$3\sqrt{7}$	$9\sqrt{15}$	$6\sqrt{21}$	$-24\sqrt{35}$	$8\sqrt{105}$	0

TABLE XVIII: Constraints on the EDF that is derived by averaging the second-order gauge-invariant pseudopotential, expressed by the formula  $C_{mI,\tilde{n}LvJ}^{n'L'v'J',1} = aC_{00,1101}^{1101,0} + bC_{00,2011}^{0011,0} + cC_{00,2211}^{0011,0} + dC_{11,0011}^{1101,0} + eC_{20,0000}^{0000,0} + fC_{20,0011}^{0011,0} + gC_{22,0011}^{0011,0}$ .

	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$C_{00,1101}^{1101,1}$	$-\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{2}{\sqrt{3}}$	-2	0
$C_{00,2011}^{0011,1}$	0	$-\frac{1}{\sqrt{3}}$	0	0	2	$-\frac{2}{\sqrt{3}}$	0
$C_{00,2211}^{0011,1}$	0	0	$-\frac{1}{\sqrt{3}}$	0	0	0	$\frac{4}{\sqrt{3}}$
$C_{11,0011}^{1101,1}$	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	0
$C_{20,0000}^{0000,1}$	$-\frac{1}{2\sqrt{3}}$	$\frac{1}{2}$	0	0	$-\frac{1}{\sqrt{3}}$	0	0
$C_{20,0011}^{0011,1}$	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{3}}$	0	0	0	$-\frac{1}{\sqrt{3}}$	0
$C_{22,0011}^{0011,1}$	0	0	$\frac{1}{\sqrt{3}}$	0	0	0	$-\frac{1}{\sqrt{3}}$

TABLE XIX: Same as in Table XVIII but for the fourth-order terms, according to the formula  $C_{mI,nLvJ}^{n'L'v'J',1} = A(aC_{00,2202}^{2202,0} + bC_{00,2212}^{2212,0} + cC_{00,4211}^{0011,0} + dC_{40,0000}^{0000,0} + eC_{40,0011}^{0011,0} + fC_{42,0011}^{0011,0})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{40,0000}^{0000,1}$	$\frac{1}{120}$	$-6\sqrt{15}$	$-18\sqrt{15}$	$-21\sqrt{5}$	$-40\sqrt{3}$	0	0
$C_{40,0011}^{0011,1}$	$\frac{1}{120}$	$-18\sqrt{5}$	$18\sqrt{5}$	$7\sqrt{15}$	0	$-40\sqrt{3}$	0
$C_{42,0011}^{0011,1}$	$-\frac{1}{\sqrt{3}}$	0	0	1	0	0	1
$C_{00,2202}^{2202,1}$	$\frac{1}{9}$	$-3\sqrt{3}$	0	0	$-4\sqrt{15}$	$-12\sqrt{5}$	0
$C_{00,4211}^{0011,1}$	$-\frac{1}{\sqrt{3}}$	0	0	1	0	0	4
$C_{00,2212}^{2212,1}$	$\frac{1}{9}$	0	$-3\sqrt{3}$	0	$-4\sqrt{15}$	$4\sqrt{5}$	14

#### IV. RELATIONS BETWEEN THE PSEUDOPOTENTIAL AND ENERGY DENSITY FUNCTIONAL WITH CONSERVED SPHERICAL SYMMETRY

In this Section, we assume the spherical, space-inversion, and time-reversal symmetries of the EDF, see Sec. IV of Ref. [2]. In this way we make our results applicable to the simplest case of spherical even-even nuclei. Below we fully show explicit results for the case of gauge symmetry conserved, whereas the full results pertaining

TABLE XX: Same as in Table XVIII but for the sixth-order terms, according to the formula  $C_{mI,nLvJ}^{n'L'v'J',1} = A(aC_{00,4212}^{2212,0} + bC_{00,3303}^{3303,0} + cC_{00,6211}^{0011,0} + dC_{60,0000}^{0000,0} + eC_{60,0011}^{0011,0} + fC_{62,0011}^{0011,0})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{60,0000}^{0000,1}$	$\frac{1}{840}$	$21\sqrt{15}$	$-45\sqrt{7}$	$126\sqrt{5}$	$-280\sqrt{3}$	0	0
$C_{60,0011}^{0011,1}$	$\frac{1}{840}$	$-21\sqrt{5}$	$-45\sqrt{21}$	$-42\sqrt{15}$	0	$-280\sqrt{3}$	0
$C_{62,0011}^{0011,1}$	$\frac{1}{\sqrt{3}}$	0	0	1	0	0	-1
$C_{00,3303}^{3303,1}$	$\frac{1}{9}$	0	$-3\sqrt{3}$	0	$-8\sqrt{7}$	$-8\sqrt{21}$	0
$C_{00,6211}^{0011,1}$	$-\frac{1}{\sqrt{3}}$	0	0	1	0	0	-4
$C_{00,4212}^{2212,1}$	$\frac{1}{3}$	$-\sqrt{3}$	0	0	$8\sqrt{15}$	$-8\sqrt{5}$	-24

TABLE XXI: Second-order coupling constants of the EDF as functions of parameters of the pseudopotential when the gauge and the spherical symmetries are simultaneously imposed, according to the formula  $C_{mI,nLvJ}^{n'L'v'J',t} = A(aC_{00,00}^{20} + bC_{00,20}^{20} + cC_{00,22}^{22} + dC_{11,00}^{11} + eC_{11,20}^{11} + fC_{11,22}^{11})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{20,0000}^{0000,0}$	$\frac{1}{32}$	-3	$-\sqrt{3}$	0	5	$-\sqrt{3}$	0
$C_{20,0000}^{0000,1}$	$\frac{1}{32}$	$\sqrt{3}$	-3	0	$\sqrt{3}$	-3	0
$C_{00,2000}^{0000,0}$	$\frac{1}{16}$	3	$\sqrt{3}$	0	5	$-\sqrt{3}$	0
$C_{00,2000}^{0000,1}$	$\frac{1}{16}$	$-\sqrt{3}$	3	0	$\sqrt{3}$	-3	0
$C_{00,1111}^{1111,0}$	$\frac{1}{48}$	3	$5\sqrt{3}$	$-\sqrt{15}$	-3	$3\sqrt{3}$	$-3\sqrt{15}$
$C_{00,1111}^{1111,1}$	$\frac{1}{16}$	$\sqrt{3}$	1	$\sqrt{5}$	$-\sqrt{3}$	-1	$-\sqrt{5}$

to the case of Galilean symmetry are given in the supplemental material [31].

When the gauge symmetry is imposed on the EDF and the isospin degree of freedom is taken into account, we have 8 independent spherical EDF terms at second order, 6 at fourth order, and 6 at sixth order. The 8 corresponding second-order coupling constants can then be expressed by the 7 second-order pseudopotential parameters. Similarly, both at fourth and sixth orders, 6 coupling constants can then be expressed by 6 pseudopotential parameters.

As is well known, at second order the isoscalar and isovector spin-orbit coupling constants depend both on one spin-orbit pseudopotential parameter, namely,

$$C_{11,1111}^{0000,0} = -\frac{3}{4}C_{11,11}^{11}, \quad (22a)$$

$$C_{11,1111}^{0000,1} = -\frac{\sqrt{3}}{4}C_{11,11}^{11}, \quad (22b)$$

which gives one constraint on the spin-orbit coupling constants,

$$C_{11,1111}^{0000,1} = \frac{1}{\sqrt{3}}C_{11,1111}^{0000,0}. \quad (23)$$

The remaining 6 spherical EDF coupling constants expressed through 6 pseudopotential parameters are given in Table XXI. Similar expressions at fourth and sixth orders are given in Tables XXII and XXIII. As in Sec. III A, from these results we can obtain the inverse expressions relating the parameters of the pseudopotential to the coupling constants of the spherical EDF; these are given in Tables XXIV–XXVI.

At second order, the gauge and Galilean symmetries are equivalent to one another [2]. When at higher orders the Galilean invariance is imposed on the spherical EDF, we have at fourth (sixth) order 18 (32) independent terms, of which 4 (8) are of the spin-orbit character. It turns out that, in the same way as for the second order, the higher-order spin-orbit coupling constants are related only to the spin-orbit pseudopotential parameters.

TABLE XXII: Same as in Table XXI but for the fourth-order coupling constants of the EDF, according to the formula  $C_{mI,nLvJ}^{n'L'v'J',t} = A(aC_{11,00}^{31} + bC_{11,20}^{31} + cC_{11,22}^{33} + dC_{22,00}^{22} + eC_{22,20}^{22} + fC_{22,22}^{22})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{40,0000}^{0000,0}$	$\frac{1}{640}$	-25	$5\sqrt{3}$	0	$18\sqrt{5}$	$6\sqrt{15}$	0
$C_{40,0000}^{0000,1}$	$\frac{1}{640}$	$-5\sqrt{3}$	15	0	$-6\sqrt{15}$	$18\sqrt{5}$	0
$C_{00,2202}^{2202,0}$	$\frac{1}{96}$	$5\sqrt{5}$	$-\sqrt{15}$	0	18	$6\sqrt{3}$	0
$C_{00,2202}^{2202,1}$	$\frac{1}{96}$	$\sqrt{15}$	$-3\sqrt{5}$	0	$-6\sqrt{3}$	18	0
$C_{00,3111}^{1111,0}$	$\frac{1}{80}$	-5	$5\sqrt{3}$	$-15\sqrt{7}$	$6\sqrt{5}$	$10\sqrt{15}$	$-2\sqrt{105}$
$C_{00,3111}^{1111,1}$	$\frac{1}{80}$	$-5\sqrt{3}$	-5	$-5\sqrt{21}$	$6\sqrt{15}$	$6\sqrt{5}$	$6\sqrt{35}$

TABLE XXIII: Same as in Table XXI but for the sixth-order coupling constants of the EDF, according to the formula  $C_{mI,nLvJ}^{n'L'v'J',t} = A(aC_{11,22}^{53} + bC_{22,00}^{42} + cC_{22,20}^{42} + dC_{22,22}^{44} + eC_{33,00}^{33} + fC_{33,20}^{33})$ .

	$A$	$a$	$b$	$c$	$d$	$e$	$f$
$C_{60,0000}^{0000,0}$	$\frac{1}{4480}$	0	$-21\sqrt{5} - 7\sqrt{15}$	0	$75\sqrt{21}$	$-45\sqrt{7}$	
$C_{60,0000}^{0000,1}$	$\frac{1}{4480}$	0	$7\sqrt{15} - 21\sqrt{5}$	0	$45\sqrt{7}$	$-45\sqrt{21}$	
$C_{00,6000}^{0000,0}$	$\frac{1}{2240}$	0	$21\sqrt{5} - 7\sqrt{15}$	0	$75\sqrt{21}$	$-45\sqrt{7}$	
$C_{00,6000}^{0000,1}$	$\frac{1}{2240}$	0	$-7\sqrt{15} - 21\sqrt{5}$	0	$45\sqrt{7}$	$-45\sqrt{21}$	
$C_{00,3111}^{3111,0}$	$\frac{1}{800}$	$-135\sqrt{7}$	$21\sqrt{5}$	$35\sqrt{15}$	$-105\sqrt{3}$	$-45\sqrt{21}$	$135\sqrt{7}$
$C_{00,3111}^{3111,1}$	$-\frac{3}{800}$	$15\sqrt{21}$	$-7\sqrt{15}$	$-7\sqrt{5}$	-105	$45\sqrt{7}$	$15\sqrt{21}$

TABLE XXIV: Second-order parameters of the pseudopotential (spin-orbit term not included) as functions of the coupling constants of the EDF when the gauge and the spherical symmetries are simultaneously imposed, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = aC_{20,0000}^{0000,0} + bC_{20,0000}^{0000,1} + cC_{00,2000}^{0000,0} + dC_{00,2000}^{0000,1} + eC_{00,1111}^{1111,0} + fC_{00,1111}^{1111,1}$ .

	$a$	$b$	$c$	$d$	$e$	$f$
$C_{00,00}^{20}$	-4	$\frac{4}{\sqrt{3}}$	2	$-\frac{2}{\sqrt{3}}$	0	0
$C_{00,20}^{20}$	$-\frac{4}{\sqrt{3}}$	-4	$\frac{2}{\sqrt{3}}$	2	0	0
$C_{00,22}^{22}$	$\frac{16}{\sqrt{15}}$	$-\frac{16}{\sqrt{5}}$	$\frac{4}{\sqrt{15}}$	$-\frac{4}{\sqrt{5}}$	$-4\sqrt{\frac{3}{5}}$	$\frac{12}{\sqrt{5}}$
$C_{11,00}^{11}$	4	$-\frac{4}{\sqrt{3}}$	2	$-\frac{2}{\sqrt{3}}$	0	0
$C_{11,20}^{11}$	$\frac{4}{\sqrt{3}}$	$-\frac{20}{3}$	$\frac{2}{\sqrt{3}}$	$-\frac{10}{3}$	0	0
$C_{11,22}^{11}$	$-\frac{16}{\sqrt{15}}$	$-\frac{16}{3\sqrt{5}}$	$\frac{4}{\sqrt{15}}$	$\frac{4}{3\sqrt{5}}$	$-4\sqrt{\frac{3}{5}}$	$-\frac{4}{\sqrt{5}}$

TABLE XXV: Fourth-order parameters of the pseudopotential as functions of the coupling constants of the EDF when the gauge and the spherical symmetries are simultaneously imposed, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = aC_{40,0000}^{0000,0} + bC_{40,0000}^{0000,1} + cC_{00,2202}^{2202,0} + dC_{00,2202}^{2202,1} + eC_{00,3111}^{1111,0} + fC_{00,3111}^{1111,1}$ .

	$a$	$b$	$c$	$d$	$e$	$f$
$C_{11,00}^{31}$	-16	$\frac{16}{\sqrt{3}}$	$\frac{12}{\sqrt{5}}$	$-4\sqrt{\frac{3}{5}}$	0	0
$C_{11,20}^{31}$	$-\frac{16}{\sqrt{3}}$	$\frac{80}{3}$	$4\sqrt{\frac{3}{5}}$	$-4\sqrt{5}$	0	0
$C_{11,22}^{33}$	$\frac{64}{3\sqrt{7}}$	$\frac{64}{3\sqrt{21}}$	$\frac{8}{\sqrt{35}}$	$\frac{8}{\sqrt{105}}$	$-\frac{4}{\sqrt{7}}$	$-\frac{4}{\sqrt{21}}$
$C_{22,00}^{22}$	$\frac{8\sqrt{5}}{3}$	$-\frac{8}{3}\sqrt{\frac{5}{3}}$	2	$-\frac{2}{\sqrt{3}}$	0	0
$C_{22,20}^{22}$	$\frac{8}{3}\sqrt{\frac{5}{3}}$	$\frac{8\sqrt{5}}{3}$	$\frac{2}{\sqrt{3}}$	2	0	0
$C_{22,22}^{22}$	$-\frac{32}{3}\sqrt{\frac{5}{21}}$	$\frac{32}{3}\sqrt{\frac{5}{7}}$	$\frac{4}{\sqrt{21}}$	$-\frac{4}{\sqrt{7}}$	$-2\sqrt{\frac{5}{21}}$	$2\sqrt{\frac{5}{7}}$

TABLE XXVI: Same as in Table XXV but for the sixth-order parameters of the pseudopotential, according to the formula  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} = aC_{60,0000}^{0000,0} + bC_{60,0000}^{0000,1} + cC_{00,6000}^{0000,0} + dC_{00,6000}^{0000,1} + eC_{00,3111}^{3111,0} + fC_{00,3111}^{3111,1}$ .

	$a$	$b$	$c$	$d$	$e$	$f$
$C_{11,22}^{53}$	$-\frac{64\sqrt{7}}{9}$	$-\frac{64}{9}\sqrt{\frac{7}{3}}$	$\frac{16\sqrt{7}}{9}$	$\frac{16}{9}\sqrt{\frac{7}{3}}$	$-\frac{40}{9\sqrt{7}}$	$-\frac{40}{9\sqrt{21}}$
$C_{22,00}^{42}$	$-16\sqrt{5}$	$16\sqrt{\frac{5}{3}}$	$8\sqrt{5}$	$-8\sqrt{\frac{5}{3}}$	0	0
$C_{22,20}^{42}$	$-16\sqrt{\frac{5}{3}}$	$-16\sqrt{5}$	$8\sqrt{\frac{5}{3}}$	$8\sqrt{5}$	0	0
$C_{22,22}^{44}$	$\frac{64}{3\sqrt{3}}$	$-\frac{64}{3}$	$\frac{16}{3\sqrt{3}}$	$-\frac{16}{3}$	$-\frac{40}{21\sqrt{3}}$	$\frac{40}{21}$
$C_{33,00}^{33}$	$\frac{16}{3}\sqrt{\frac{7}{3}}$	$-\frac{16\sqrt{7}}{9}$	$\frac{8}{3}\sqrt{\frac{7}{3}}$	$-\frac{8}{9}\sqrt{7}$	0	0
$C_{33,20}^{33}$	$\frac{16\sqrt{7}}{9}$	$-\frac{80}{9}\sqrt{\frac{7}{3}}$	$\frac{8\sqrt{7}}{9}$	$-\frac{40}{9}\sqrt{\frac{7}{3}}$	0	0

ters. Namely, at fourth order we have

$$C_{31,1111}^{0000,0} = \frac{3}{16}C_{11,11}^{31} - \frac{1}{8}\sqrt{\frac{3}{5}}C_{22,11}^{22}, \quad (24a)$$

$$C_{31,1111}^{0000,1} = \frac{1}{16}\sqrt{3}C_{11,11}^{31} + \frac{3}{8}\sqrt{\frac{1}{5}}C_{22,11}^{22}, \quad (24b)$$

$$C_{11,3111}^{0000,0} = -\frac{3}{16}C_{11,11}^{31} - \frac{1}{8}\sqrt{\frac{3}{5}}C_{22,11}^{22}, \quad (24c)$$

$$C_{11,3111}^{0000,1} = -\frac{1}{16}\sqrt{3}C_{11,11}^{31} + \frac{3}{8}\sqrt{\frac{1}{5}}C_{22,11}^{22}, \quad (24d)$$

which gives the following constraints on the spin-orbit coupling constants:

$$C_{31,1111}^{0000,1} = -\frac{1}{\sqrt{3}}C_{31,1111}^{0000,0} - \frac{2}{\sqrt{3}}C_{11,3111}^{0000,0}, \quad (25a)$$

$$C_{11,3111}^{0000,1} = -\frac{2}{\sqrt{3}}C_{31,1111}^{0000,0} - \frac{1}{\sqrt{3}}C_{11,3111}^{0000,0}, \quad (25b)$$

and at sixth order we have

$$C_{51,1111}^{0000,0} = -\frac{3}{64}C_{11,11}^{51} + \frac{1}{32}\sqrt{\frac{3}{5}}C_{22,11}^{42} - \frac{3}{64}C_{31,11}^{31} - \frac{27}{80}\sqrt{\frac{1}{14}}C_{33,11}^{33}, \quad (26a)$$

$$C_{51,1111}^{0000,1} = -\frac{\sqrt{3}}{64}C_{11,11}^{51} - \frac{3}{32}\sqrt{\frac{1}{5}}C_{22,11}^{42} - \frac{\sqrt{3}}{64}C_{31,11}^{31} - \frac{9}{80}\sqrt{\frac{3}{14}}C_{33,11}^{33}, \quad (26b)$$

$$C_{11,5111}^{0000,0} = -\frac{3}{64}C_{11,11}^{51} - \frac{1}{32}\sqrt{\frac{3}{5}}C_{22,11}^{42} - \frac{3}{64}C_{31,11}^{31} - \frac{27}{80}\sqrt{\frac{1}{14}}C_{33,11}^{33}, \quad (26c)$$

$$C_{11,5111}^{0000,1} = -\frac{\sqrt{3}}{64}C_{11,11}^{51} + \frac{3}{32}\sqrt{\frac{1}{5}}C_{22,11}^{42} - \frac{\sqrt{3}}{64}C_{31,11}^{31} - \frac{9}{80}\sqrt{\frac{3}{14}}C_{33,11}^{33}, \quad (26d)$$

$$C_{31,3111}^{0000,0} = \frac{21}{160}C_{11,11}^{51} + \frac{9}{160}C_{31,11}^{31} - \frac{27}{200}\sqrt{\frac{7}{2}}C_{33,11}^{33}, \quad (26e)$$

$$C_{31,3111}^{0000,1} = \frac{7}{160}\sqrt{3}C_{11,11}^{51} + \frac{3}{160}\sqrt{3}C_{31,11}^{31} - \frac{9}{200}\sqrt{\frac{21}{2}}C_{33,11}^{33}, \quad (26f)$$

$$C_{33,3313}^{0000,0} = \frac{1}{24}\sqrt{\frac{7}{2}}C_{11,11}^{51} - \frac{1}{24}\sqrt{\frac{7}{2}}C_{31,11}^{31} + \frac{3}{80}C_{33,11}^{33}, \quad (26g)$$

$$C_{33,3313}^{0000,1} = \frac{1}{24}\sqrt{\frac{7}{6}}C_{11,11}^{51} - \frac{1}{24}\sqrt{\frac{7}{6}}C_{31,11}^{31} + \frac{\sqrt{3}}{80}C_{33,11}^{33}, \quad (26h)$$

which gives the constraints:

$$C_{51,1111}^{0000,1} = -\frac{1}{\sqrt{3}}C_{51,1111}^{0000,0} + \frac{2}{\sqrt{3}}C_{11,5111}^{0000,0}, \quad (27a)$$

$$C_{11,5111}^{0000,1} = \frac{2}{\sqrt{3}}C_{51,1111}^{0000,0} - \frac{1}{\sqrt{3}}C_{11,5111}^{0000,0}, \quad (27b)$$

$$C_{31,3111}^{0000,1} = \frac{1}{\sqrt{3}}C_{31,3111}^{0000,0}, \quad (27c)$$

$$C_{33,3313}^{0000,1} = \frac{1}{\sqrt{3}}C_{33,3313}^{0000,0}. \quad (27d)$$

If now we consider the Galilean-invariant and spherical EDF without spin-orbit terms, we obtain at fourth (sixth) order 1 (2) possible constraints among the remaining 14 (24) coupling constants related to the remaining 13 (22) parameters of the pseudopotential. These results are available in the supplemental material [31]. Of course, such constraints can be imposed in very many

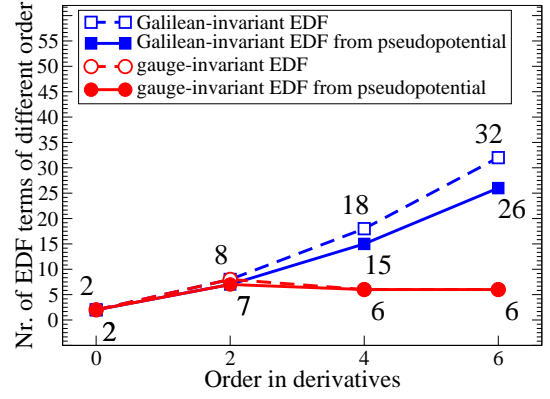


FIG. 2: (Color online) Number of terms of the spherical EDF that is related to a pseudopotential (solid lines). Full squares and circles show results for the Galilean and gauge invariance, respectively. For reference, dashed lines with open squares and circles show the corresponding results for the general spherical EDF studied in Ref. [2].

different ways. We have checked that, in fact, not any of the 1 (2) coupling constants of the fourth (sixth) order spherical EDF can be considered as being dependent on all the other coupling constants. In the supplemental material we present one example of a possible choice, whereby at fourth (sixth) order the coupling constants  $C_{22,1111}^{1111,1}$  ( $C_{00,3111}^{3111,0}$  and  $C_{00,3111}^{3111,1}$ ) are selected to be dependent. A comparison between the numbers of terms of the Galilean-invariant and gauge-invariant spherical EDF with and without constraints coming from the reference to the pseudopotential is plotted in Fig. 2.

## V. CONCLUSIONS

In summary, in this work we derived the Galilean-invariant nuclear  $N^3$ LO pseudopotential with derivatives up to sixth order and found the corresponding  $N^3$ LO EDF, which was obtained by calculating the corresponding HF average energy. Owing to the zero range of the pseudopotential, the number of terms thereof is twice smaller than that of the most general EDF. We found explicit linear relations between the parameters of the pseudopotential and coupling constant of the EDF. These linear relations constitute a set of constraints, which allow for expressing one half of the coupling constants through the other half. As an example of such constraints, we have derived linear relations between the isoscalar and isovector coupling constants. The gauge-invariant form of the pseudopotential was also derived, and all derivations were repeated also for this case.

We have also analyzed properties of the EDF restricted by imposing the spherical, space-inversion, and time-reversal symmetries, which are relevant for describing spherical nuclei. In this case, by relating the EDF to the pseudopotential, at second, fourth, and sixth order one reduces the numbers of coupling constants only from

TABLE XXVII: Number of terms of different orders in the pseudopotential (2) and in the EDF up to  $N^3\text{LO}$ , evaluated for the conserved Galilean and gauge symmetries. The last four columns show the number of terms in the EDF evaluated by taking into account the additional constraints coming from the relation of the EDF to pseudopotential.

Order	Pseudopotential		EDF							
	Galilean	Gauge	Not related to pseudopotential				Related to pseudopotential			
			General		Spherical		General		Spherical	
	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge
0	2	2	4	4	2	2	2	2	2	2
2	7	7	14	14	8	8	7	7	7	7
4	15	6	30	12	18	6	15	6	15	6
6	26	6	52	12	32	6	26	6	26	6
$N^3\text{LO}$	50	21	100	42	60	22	50	21	50	21

8, 18, and 32 to 7, 15, and 26, respectively. Such reduction has two origins: (i) at each order 1, 2, or 4 spin-orbit isovector and isoscalar coupling constants become dependent on one another and (ii) at fourth and sixth order one or two non-spin-orbit coupling constants become linearly dependent on the remaining 13 or 22 ones, respectively. Therefore, in spherical magic nuclei one can expect relatively small effects related to imposing on the EDF the pseudopotential origins, whereas this may have much more important consequences in deformed, asymmetric, odd, and/or rotating nuclei. We also note that for the EDF related to pseudopotential, imposing the spherical symmetry does not change the numbers of independent coupling constants as compared to the general case.

Table XXVII gives an overview of the results by showing the number of terms of pseudopotential and EDF with Galilean or gauge symmetries imposed.

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### Appendix A: Time-reversal invariance and hermiticity of the pseudopotential

The pseudopotential studied in this work is a contact interaction built with derivative and spin operators. Furthermore, the choice concerning the formalism is the use of the spherical tensors. Under these assumptions, the general structure of the pseudopotential is based on the following building blocks,

$$\hat{V}_0 = \left[ [K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}]_S \hat{S}_{v_{12}S} \right]_0 \hat{\delta}_{12}(\mathbf{r}'_1 \mathbf{r}'_2; \mathbf{r}_1 \mathbf{r}_2). \quad (\text{A1})$$

The final coupling to a scalar ensures that  $\hat{V}_0$  is invariant under space rotation. Moreover, provided that  $\tilde{n}' + \tilde{n}$  is even, it is also invariant under space-inversion. Now we proceed to explore another fundamental symmetry, the time-reversal, and later we also require the hermiticity of the pseudopotential.

The time-reversal operator  $\hat{T} = -i\sigma_y \hat{K}$ , where  $\hat{K}$  is the complex conjugation in space representation, can be explicitly applied to the spherical-tensor representations of momentum and spin operators, Eqs. (3), (5), and (6), which gives the generic result for spherical tensors,

$$\hat{T} A_{\lambda\mu} \hat{T}^\dagger = T_A (-1)^{\lambda-\mu} A_{\lambda,-\mu}, \quad (\text{A2})$$

where  $T_A$  are numerical phase factors. In our case, we obtain  $T_k = -1$  for the momentum operator and  $T_{\sigma_v} = (-1)^v$  for the scalar ( $v = 0$ ) and vector ( $v = 1$ ) spin operators. Moreover, since the Clebsch-Gordan coefficients are real, rule (A2) propagates through the angular momentum coupling, that is, if phase factors  $T_A$  and  $T_{A'}$  characterize tensors  $A_\lambda$  and  $A'_{\lambda'}$ , respectively, then the coupled tensor,

$$A''_{\lambda''\mu''} = [A_\lambda A'_{\lambda'}]_{\lambda''\mu''} = \sum_{\mu\mu'} C_{\lambda\mu\lambda'\mu'}^{\lambda''\mu''} A_{\lambda\mu} A'_{\lambda'\mu'}, \quad (\text{A3})$$

is characterized by the product of phase factors  $T_{A''} = T_A T_{A'}$  (cf. Appendix B in Ref. [2]). Therefore, the coupled operators appearing in  $\hat{V}_0$  (A1) are characterized by the following values of phase factors,

$$T_{K'_{\tilde{n}'\tilde{L}'}} = (-1)^{\tilde{n}'}, \quad (\text{A4a})$$

$$T_{K_{\tilde{n}\tilde{L}}} = (-1)^{\tilde{n}}, \quad (\text{A4b})$$

$$T_{S_{v_{12}S}} = (-1)^{v_{12}}. \quad (\text{A4c})$$

Finally, because the Dirac delta is real, for  $\hat{V}_0$  we have,

$$T_{\hat{V}_0} = (-1)^{\tilde{n}' + \tilde{n} + v_{12}}, \quad (\text{A5})$$

and by taking into account the space-inversion invariance, it boils down to

$$T_{\hat{V}_0} = (-1)^{v_{12}}. \quad (\text{A6})$$

This justifies the phase factor  $i^{v_{12}}$  in the definition of the pseudopotential in Eq. (2), which ensures that for real parameters, all terms of the pseudopotential are time-even.

Now we can proceed to calculate the adjoint of the operator  $\hat{V}_0$  (A1) multiplied by the phase factor derived above, that is,

$$\left(i^{v_{12}}\hat{V}_0\right)^\dagger = (-i)^{v_{12}} \left[ [K_{\tilde{n}'\tilde{L}'}K'_{\tilde{n}\tilde{L}}]_S^* \hat{S}_{v_{12}S}^\dagger \right]_0 \hat{\delta}_{12}(\mathbf{r}'_1\mathbf{r}'_2; \mathbf{r}_1\mathbf{r}_2), \quad (\text{A7})$$

where we treat the space derivatives of the Dirac delta like ordinary numbers and the space variables had to be exchanged,  $\mathbf{r}'_1 \leftrightarrow \mathbf{r}_1$  and  $\mathbf{r}'_2 \leftrightarrow \mathbf{r}_2$ .

Properties of generic spherical tensors under the complex and Hermitian conjugations are given by the following rules,

$$A_{\lambda\mu}^* = P_A(-1)^{\lambda-\mu} A_{\lambda,-\mu}, \quad (\text{A8})$$

$$A_{\lambda\mu}^\dagger = H_A(-1)^{\lambda-\mu} A_{\lambda,-\mu}, \quad (\text{A9})$$

where the phase factors  $P_A$  and  $H_A$  can be directly derived from definitions (3), (5), and (6), that is,  $P_k = -1$  and  $H_{\sigma_v} = +1$ . These rules also propagate through the angular momentum coupling, that is,  $P_{A''} = P_A P_{A'}$  and, for *commuting operators*, which is the case here,  $H_{A''} = H_A H_{A'}$ . Therefore, we have,

$$P_{[K_{\tilde{n}'\tilde{L}'}K'_{\tilde{n}\tilde{L}}]_S} = (-1)^{\tilde{n}'+\tilde{n}} = +1, \quad (\text{A10})$$

and

$$H_{\hat{S}_{v_{12}S}} = +1. \quad (\text{A11})$$

Finally, the adjoint operator of Eq. (A7) is given by

$$\left(i^{v_{12}}\hat{V}_0\right)^\dagger = (-i)^{v_{12}} \left[ [K_{\tilde{n}'\tilde{L}'}K'_{\tilde{n}\tilde{L}}]_S \hat{S}_{v_{12}S} \right]_0 \hat{\delta}_{12}(\mathbf{r}'_1\mathbf{r}'_2; \mathbf{r}_1\mathbf{r}_2) = i^{v_{12}}(-1)^{v_{12}+S} \left[ [K'_{\tilde{n}\tilde{L}}K_{\tilde{n}'\tilde{L}'}]_S \hat{S}_{v_{12}S} \right]_0 \hat{\delta}_{12}(\mathbf{r}'_1\mathbf{r}'_2; \mathbf{r}_1\mathbf{r}_2), \quad (\text{A12})$$

where the last equality results from flipping the order of coupling of the operators  $K_{\tilde{n}'\tilde{L}'}$  and  $K'_{\tilde{n}\tilde{L}}$ , which brings out the phase factor of  $(-1)^{S-\tilde{L}'-\tilde{L}} = (-1)^S$ . Therefore, the time-even tensor  $i^{v_{12}}\hat{V}_0$  is not self-adjoint, but we can hermitize it by using the expression given in Eq. (2).

## Appendix B: Relations defining the gauge-invariant pseudopotentials

As discussed in Section II C, when the gauge invariance is imposed on the pseudopotential, one obtains a specific set of constraints on the parameters and terms of the pseudopotential, which result from the condition of Eq. (13).

At fourth order, the gauge symmetry forces seven parameters of terms listed in the Table IV to be specific linear combinations of the four independent ones, namely,

$$C_{00,00}^{40} = \frac{3}{2\sqrt{5}} C_{22,00}^{22}, \quad (\text{B1})$$

$$C_{00,20}^{40} = \frac{3}{2\sqrt{5}} C_{22,20}^{22}, \quad (\text{B2})$$

$$C_{00,22}^{42} = \frac{3}{\sqrt{7}} C_{22,22}^{22}, \quad (\text{B3})$$

$$C_{11,22}^{31} = \sqrt{\frac{21}{5}} C_{11,22}^{33}, \quad (\text{B4})$$

$$C_{20,00}^{20} = \frac{\sqrt{5}}{2} C_{22,00}^{22}, \quad (\text{B5})$$

$$C_{20,20}^{20} = \frac{\sqrt{5}}{2} C_{22,20}^{22}, \quad (\text{B6})$$

$$C_{20,22}^{22} = \sqrt{7} C_{22,22}^{22}. \quad (\text{B7})$$

At sixth order, imposing the gauge symmetry forces 16 terms of the pseudopotential listed in Table V to be specific linear combinations of 6 independent ones, namely,

$$C_{00,00}^{60} = \frac{1}{4\sqrt{5}} C_{22,00}^{42}, \quad (\text{B8})$$

$$C_{00,20}^{60} = \frac{1}{4\sqrt{5}} C_{22,20}^{42}, \quad (\text{B9})$$

$$C_{00,22}^{62} = \frac{\sqrt{5}}{4} C_{22,22}^{44}, \quad (\text{B10})$$

$$C_{11,00}^{51} = \frac{9}{2} \sqrt{\frac{3}{7}} C_{33,00}^{33}, \quad (\text{B11})$$

$$C_{11,20}^{51} = \frac{9}{2} \sqrt{\frac{3}{7}} C_{33,20}^{33}, \quad (\text{B12})$$

$$C_{11,22}^{51} = \frac{9}{2} \sqrt{\frac{3}{35}} C_{11,22}^{53}, \quad (\text{B13})$$

$$C_{20,00}^{40} = \frac{7}{4\sqrt{5}} C_{22,00}^{42}, \quad (\text{B14})$$

$$C_{20,20}^{40} = \frac{7}{4\sqrt{5}} C_{22,20}^{42}, \quad (\text{B15})$$

$$C_{20,22}^{42} = \frac{3\sqrt{5}}{2} C_{22,22}^{44}, \quad (\text{B16})$$

$$C_{22,22}^{40} = \frac{21}{4\sqrt{5}} C_{22,22}^{44}, \quad (\text{B17})$$

$$C_{22,22}^{42} = 3\sqrt{\frac{5}{7}} C_{22,22}^{44}, \quad (\text{B18})$$

$$C_{31,00}^{31} = \frac{9}{10} \sqrt{21} C_{33,00}^{33}, \quad (\text{B19})$$

$$C_{31,20}^{31} = \frac{9}{10} \sqrt{21} C_{33,20}^{33}, \quad (\text{B20})$$

$$C_{31,22}^{31} = \frac{9}{10} \sqrt{\frac{21}{5}} C_{11,22}^{53}, \quad (\text{B21})$$

$$C_{31,22}^{33} = \frac{9}{5} C_{11,22}^{53}, \quad (\text{B22})$$

$$C_{33,22}^{33} = \sqrt{\frac{2}{15}} C_{11,22}^{53}. \quad (\text{B23})$$

### Appendix C: Relations between the central-like and tensor-like pseudopotentials

In the following we present the recoupling formulae which connect the two alternative forms of the pseudopotential of the Eqs. (1) and (14). We have,

$$\begin{aligned} \hat{V}_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} &= \frac{1}{2} i^{v_{12}} (1 - \frac{1}{2} \delta_{v_1,v_2}) \sqrt{2S+1} \\ &\times \left( \sum_{J=|\tilde{L}'-v_1|}^{\tilde{L}'+v_1} (-1)^{J+S+v_1+\tilde{L}} \sqrt{2J+1} \begin{Bmatrix} \tilde{L}' & v_1 & J \\ v_2 & \tilde{L} & S \end{Bmatrix} \left[ [K'_{\tilde{n}'\tilde{L}'} \sigma_{v_1}^{(1)}]_J [K_{\tilde{n}\tilde{L}} \sigma_{v_2}^{(2)}]_J \right]_0 \right. \\ &+ \sum_{J=|\tilde{L}'-v_1|}^{\tilde{L}'+v_1} (-1)^{J+v_2+\tilde{L}} \sqrt{2J+1} \begin{Bmatrix} \tilde{L}' & v_1 & J \\ v_2 & \tilde{L} & S \end{Bmatrix} \left[ [K'_{\tilde{n}'\tilde{L}'} \sigma_{v_1}^{(2)}]_J [K_{\tilde{n}\tilde{L}} \sigma_{v_2}^{(1)}]_J \right]_0 \\ &+ \sum_{J=|\tilde{L}-v_1|}^{\tilde{L}+v_1} (-1)^{J+v_2+\tilde{L}'} \sqrt{2J+1} \begin{Bmatrix} \tilde{L} & v_1 & J \\ v_2 & \tilde{L}' & S \end{Bmatrix} \left[ [K'_{\tilde{n}\tilde{L}} \sigma_{v_1}^{(1)}]_J [K_{\tilde{n}'\tilde{L}'} \sigma_{v_2}^{(2)}]_J \right]_0 \\ &+ \sum_{J=|\tilde{L}-v_1|}^{\tilde{L}+v_1} (-1)^{J+S+v_1+\tilde{L}'} \sqrt{2J+1} \begin{Bmatrix} \tilde{L} & v_1 & J \\ v_2 & \tilde{L}' & S \end{Bmatrix} \left[ [K'_{\tilde{n}\tilde{L}} \sigma_{v_1}^{(2)}]_J [K_{\tilde{n}'\tilde{L}'} \sigma_{v_2}^{(1)}]_J \right]_0 \Bigg) \\ &\times \left( 1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \hat{\delta}_{12}(\mathbf{r}'_1 \mathbf{r}'_2; \mathbf{r}_1 \mathbf{r}_2). \end{aligned} \quad (\text{C1})$$

Analogously, the recoupling formula which allows to express the tensor-like pseudopotential through the central-like

one reads,

$$\begin{aligned}
\hat{V}_{\tilde{n}\tilde{L},v_{12}J}^{\tilde{n}'\tilde{L}'} &= \frac{1}{2}i^{v_{12}} \left(1 - \frac{1}{2}\delta_{v_1,v_2}\right) \sqrt{2J+1} \sum_{S=|\tilde{L}'-\tilde{L}|}^{\tilde{L}'+\tilde{L}} \sqrt{2S+1} \\
&\times \left( (-1)^{S+J+v_1+\tilde{L}} \begin{Bmatrix} \tilde{L}' & \tilde{L} & S \\ v_2 & v_1 & J \end{Bmatrix} \left[ [K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}]_S \left[ \sigma_{v_1}^{(1)} \sigma_{v_2}^{(2)} \right]_S \right]_0 \right. \\
&+ (-1)^{J+v_2+\tilde{L}} \begin{Bmatrix} \tilde{L}' & \tilde{L} & S \\ v_2 & v_1 & J \end{Bmatrix} \left[ [K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}]_S \left[ \sigma_{v_2}^{(1)} \sigma_{v_1}^{(2)} \right]_S \right]_0 \\
&+ (-1)^{S+J+v_1+\tilde{L}'} \begin{Bmatrix} \tilde{L} & \tilde{L}' & S \\ v_2 & v_1 & J \end{Bmatrix} \left[ [K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'}]_S \left[ \sigma_{v_1}^{(1)} \sigma_{v_2}^{(2)} \right]_S \right]_0 \\
&+ (-1)^{J+v_2+\tilde{L}'} \begin{Bmatrix} \tilde{L} & \tilde{L}' & S \\ v_2 & v_1 & J \end{Bmatrix} \left[ [K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'}]_S \left[ \sigma_{v_2}^{(1)} \sigma_{v_1}^{(2)} \right]_S \right]_0 \Big) \\
&\times \left( 1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta_{12}(\mathbf{r}'_1 \mathbf{r}'_2; \mathbf{r}_1 \mathbf{r}_2).
\end{aligned} \tag{C2}$$

According to the recoupling of the Eq. (C1), we give the list of the relations between the parameters of the two forms of the pseudopotential. For the second order terms we have,

$$C_{00,00}^{20} = \tilde{C}_{00,00}^{20}, \tag{C3}$$

$$C_{00,20}^{20} = \tilde{C}_{00,21}^{20}, \tag{C4}$$

$$C_{00,22}^{22} = \tilde{C}_{00,21}^{22}, \tag{C5}$$

$$C_{11,00}^{11} = \tilde{C}_{11,01}^{11}, \tag{C6}$$

$$C_{11,20}^{11} = \frac{1}{3}\tilde{C}_{11,20}^{11} + \frac{1}{\sqrt{3}}\tilde{C}_{11,21}^{11} + \frac{\sqrt{5}}{3}\tilde{C}_{11,22}^{11}, \tag{C7}$$

$$C_{11,11}^{11} = -\tilde{C}_{11,11}^{11}, \tag{C8}$$

$$C_{11,22}^{11} = \frac{\sqrt{5}}{3}\tilde{C}_{11,20}^{11} - \frac{\sqrt{5}}{2\sqrt{3}}\tilde{C}_{11,21}^{11} + \frac{1}{6}\tilde{C}_{11,22}^{11}; \tag{C9}$$

at the fourth order,

$$C_{00,00}^{40} = \tilde{C}_{00,00}^{40}, \tag{C10}$$

$$C_{00,20}^{40} = \tilde{C}_{00,21}^{40}, \tag{C11}$$

$$C_{00,22}^{42} = \tilde{C}_{00,21}^{42}, \tag{C12}$$

$$C_{11,00}^{31} = \tilde{C}_{11,01}^{31}, \tag{C13}$$

$$C_{11,20}^{31} = \frac{1}{3}\tilde{C}_{11,20}^{31} + \frac{1}{\sqrt{3}}\tilde{C}_{11,21}^{31} + \frac{\sqrt{5}}{3}\tilde{C}_{11,22}^{31}, \tag{C14}$$

$$C_{11,11}^{31} = -\tilde{C}_{11,11}^{31}, \tag{C15}$$

$$C_{11,22}^{31} = \frac{\sqrt{5}}{3}\tilde{C}_{11,20}^{31} - \frac{\sqrt{5}}{2\sqrt{3}}\tilde{C}_{11,21}^{31} + \frac{1}{6}\tilde{C}_{11,22}^{31}, \tag{C16}$$

$$C_{11,22}^{33} = \tilde{C}_{11,22}^{33}, \tag{C17}$$

$$C_{20,00}^{20} = \tilde{C}_{20,00}^{20}, \tag{C18}$$

$$C_{20,20}^{20} = \tilde{C}_{20,21}^{20}, \tag{C19}$$

$$C_{20,22}^{22} = \tilde{C}_{20,21}^{22}, \tag{C20}$$

$$C_{22,00}^{22} = \tilde{C}_{22,02}^{22}, \tag{C21}$$

$$C_{22,20}^{22} = \frac{1}{\sqrt{5}}\tilde{C}_{22,21}^{22} + \frac{1}{\sqrt{3}}\tilde{C}_{22,22}^{22} + \sqrt{\frac{7}{15}}\tilde{C}_{22,23}^{22}, \tag{C22}$$

$$C_{22,11}^{22} = -\tilde{C}_{22,12}^{22}, \tag{C23}$$

$$C_{22,22}^{22} = \frac{\sqrt{35}}{10}\tilde{C}_{22,21}^{22} - \frac{\sqrt{7}}{2\sqrt{3}}\tilde{C}_{22,22}^{22} + \frac{1}{\sqrt{15}}\tilde{C}_{22,23}^{22}; \tag{C24}$$

at the sixth order,

$$C_{00,00}^{60} = \tilde{C}_{00,00}^{60}, \tag{C25}$$

$$C_{00,20}^{60} = \tilde{C}_{00,21}^{60}, \tag{C26}$$

$$C_{00,22}^{62} = \tilde{C}_{00,21}^{62}, \tag{C27}$$



$$C_{11,00}^{51} = \tilde{C}_{11,01}^{51}, \quad (C28)$$

$$C_{22,22}^{44} = \tilde{C}_{22,23}^{44}, \quad (C41)$$

$$C_{11,20}^{51} = \frac{1}{3}\tilde{C}_{11,20}^{51} + \frac{1}{\sqrt{3}}\tilde{C}_{11,21}^{51} + \frac{\sqrt{5}}{3}\tilde{C}_{11,22}^{51}, \quad (C29)$$

$$C_{31,00}^{31} = \tilde{C}_{31,01}^{31}, \quad (C42)$$

$$C_{11,11}^{51} = -\tilde{C}_{11,11}^{51}, \quad (C30)$$

$$C_{31,20}^{31} = \frac{1}{3}\tilde{C}_{31,20}^{31} + \frac{1}{\sqrt{3}}\tilde{C}_{31,21}^{31} + \frac{\sqrt{5}}{3}\tilde{C}_{31,22}^{31}, \quad (C43)$$

$$C_{11,22}^{51} = \frac{\sqrt{5}}{3}\tilde{C}_{11,20}^{51} - \frac{\sqrt{5}}{2\sqrt{3}}\tilde{C}_{11,21}^{51} + \frac{1}{6}\tilde{C}_{11,22}^{51}, \quad (C31)$$

$$C_{31,11}^{31} = -\tilde{C}_{31,11}^{31}, \quad (C44)$$

$$C_{11,22}^{53} = \tilde{C}_{11,22}^{53}, \quad (C32)$$

$$C_{20,00}^{40} = \tilde{C}_{20,00}^{40}, \quad (C33)$$

$$C_{31,22}^{31} = \frac{\sqrt{5}}{3}\tilde{C}_{31,20}^{31} - \frac{\sqrt{5}}{2\sqrt{3}}\tilde{C}_{31,21}^{31} + \frac{1}{6}\tilde{C}_{31,22}^{31}, \quad (C45)$$

$$C_{20,20}^{40} = \tilde{C}_{20,21}^{40}, \quad (C34)$$

$$C_{31,22}^{33} = \tilde{C}_{31,22}^{33}, \quad (C46)$$

$$C_{20,22}^{42} = \tilde{C}_{20,21}^{42}, \quad (C35)$$

$$C_{33,00}^{33} = \tilde{C}_{33,03}^{33}, \quad (C47)$$

$$C_{22,22}^{40} = \tilde{C}_{22,21}^{40}, \quad (C36)$$

$$C_{22,00}^{42} = \tilde{C}_{22,02}^{42}, \quad (C37)$$

$$C_{33,20}^{33} = \sqrt{\frac{5}{21}}\tilde{C}_{33,22}^{33} + \frac{1}{\sqrt{3}}\tilde{C}_{33,23}^{33} + \sqrt{\frac{3}{7}}\tilde{C}_{33,24}^{33}, \quad (C48)$$

$$C_{22,20}^{42} = \frac{1}{\sqrt{5}}\tilde{C}_{22,21}^{42} + \frac{1}{\sqrt{3}}\tilde{C}_{22,22}^{42} + \sqrt{\frac{7}{15}}\tilde{C}_{22,23}^{42}, \quad (C38)$$

$$C_{33,11}^{33} = -\tilde{C}_{33,13}^{33}, \quad (C49)$$

$$C_{22,11}^{42} = -\tilde{C}_{22,12}^{42}, \quad (C39)$$

$$C_{33,22}^{33} = \sqrt{\frac{2}{7}}\tilde{C}_{33,22}^{33} - \frac{\sqrt{5}}{2\sqrt{2}}\tilde{C}_{33,23}^{33} + \frac{\sqrt{5}}{2\sqrt{14}}\tilde{C}_{33,24}^{33}. \quad (C50)$$

$$C_{22,22}^{42} = \frac{\sqrt{35}}{10}\tilde{C}_{22,21}^{42} - \frac{\sqrt{7}}{2\sqrt{3}}\tilde{C}_{22,22}^{42} + \frac{1}{\sqrt{15}}\tilde{C}_{22,23}^{42}, \quad (C40)$$

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